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L1 44 S MALDI AND ((DETECTION OR IONIZATION) (3A) EFFICIEN?)

L2 1 S L1 AND CALIBRATION?

L1 ANSWER 1 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2003:184260 CAPLUS

TITLE: Syntheses of isotope-labeled and unlabeled iodoacetanilide and application to quantitative analysis of peptides by stable isotope differential mass spectrometry

AUTHOR(S): Niwayama, Satomi; Kurono, Sadamu; Matsumoto, Hiroyuki

CORPORATE SOURCE: Department of Chemistry, Oklahoma State University, Stillwater, OK, 74078-3071, USA

SOURCE: Abstracts of Papers, 225th ACS National Meeting, New Orleans, LA, United States, March 23-27, 2003 (2003), MEDI-294. American Chemical Society: Washington, D. C.

CODEN: 69DSA4

DOCUMENT TYPE: Conference; Meeting Abstract

LANGUAGE: English

AB Quant. anal. of proteins is very important to proteomics research. Iodoacetamide is known to specifically modify terminal SH groups of cysteine residues in proteins. In our ongoing study for development of a methodol. for quant. anal. of proteins within a complex protein mixt. for proteomics research, we synthesized a set of <sup>13</sup>C-labeled and -unlabeled iodoacetanilides, which have the same reactivity as iodoacetamide. The mol. wt. of isotope-labeled iodoacetanilide is 6 Da greater than that of the unlabeled iodoacetanilide. Our methodol. allows use of MALDI -TOF mass spectrometry for analyzing the relative quantities of peptides modified by the isotope-labeled or -unlabeled iodoacetanilide, as these derivs. are expected to exhibit identical ionization efficiencies as well as chem. reactivities. In order to test their applicability, we reacted this set of reagents with several peptides and confirmed that quant. anal. of peptides is possible.

L1 ANSWER 2 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2003:182249 CAPLUS

TITLE: Aerosol MALDI for real-time detection of bioaerosols

AUTHOR(S): Jackson, Shelley N.; Mishra, Sushama; Murray, Kermit K.

CORPORATE SOURCE: Department of Chemistry, Louisiana State University, Baton Rouge, LA, 70803, USA

SOURCE: Abstracts of Papers, 225th ACS National Meeting, New Orleans, LA, United States, March 23-27, 2003 (2003), ENVR-177. American Chemical Society: Washington, D. C.

CODEN: 69DSA4

DOCUMENT TYPE: Conference; Meeting Abstract

LANGUAGE: English

AB The threat of aerosol-borne biol. warfare agents as well as the public

health concerns assocd. with bioaerosols has led to a crucial need for real-time bioaerosol detection methods. The goal of this research is to develop an instrument for real-time anal. of bioaerosols by online single particle matrix assisted laser desorption/ionization (MALDI). In our approach, matrix is added to bioaerosols by condensation and the matrix-coated particles are ionized by pulsed UV laser radiation for mass sepn. in a TOF mass spectrometer. We have recently demonstrated enhanced ionization efficiency of large mols. in deposited aerosol particles using matrix addn. by condensation. Expts. are underway to couple matrix coating to the single particle mass spectrometer.

L1 ANSWER 3 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2003:178798 CAPLUS

TITLE: Two-laser IR/UV matrix-assisted laser desorption ionization

AUTHOR(S): Little, Mark W.; Kim, Jae-Kuk; Murray, Kermit K.

CORPORATE SOURCE: Department of Chemistry, Louisiana State University, Baton Rouge, LA, 70803-1804, USA

SOURCE: Abstracts of Papers, 225th ACS National Meeting, New Orleans, LA, United States, March 23-27, 2003 (2003), ANYL-089. American Chemical Society: Washington, D. C.

CODEN: 69DSA4

DOCUMENT TYPE: Conference; Meeting Abstract

LANGUAGE: English

AB We have developed a novel two-laser matrix-assisted laser desorption ionization (L2-MALDI) technique. The technique involves ablating a quantity of sample with an IR laser followed by UV laser irradian. of the same sample spot after an adjustable delay time. Previous two-pulse and two-laser MALDI techniques have only employed a single wavelength. We are using this technique both to study the fundamental processes of MALDI ion formation as well as for improved ionization efficiency. We have found that the UV MALDI ionization efficiency can be enhanced if the sample is first irradiated with a 10.6  $\mu\text{m}$  CO<sub>2</sub> laser, followed within 1 and 100  $\mu\text{s}$  by a 337 nm N<sub>2</sub> laser. These studies are being extended to 3  $\mu\text{m}$  / 337 nm L2-MALDI and applications with direct gel and tissue anal.

L1 ANSWER 4 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2003:119142 CAPLUS

TITLE: Bacteriocin detection from whole bacteria by matrix-assisted laser desorption ionization-time of flight mass spectrometry

AUTHOR(S): Hindre, Thomas; Didelot, Sandrine; Le Pennec, Jean-Paul; Haras, Dominique; Dufour, Alain; Vallee-Rehel, Karine

CORPORATE SOURCE: Laboratoire de Biologie et Chimie Moleculaires, EA 2594, Universite de Bretagne Sud, Lorient, 56321, Fr.

SOURCE: Applied and Environmental Microbiology (2003), 69(2), 1051-1058

CODEN: AEMIDF; ISSN: 0099-2240

PUBLISHER: American Society for Microbiology

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Class I bacteriocins (lantibiotics) and class II bacteriocins are antimicrobial peptides secreted by gram-pos. bacteria. Using two lantibiotics, lacticin 481 and nisin, and the class II bacteriocin coagulin, we showed that bacteriocins can be detected without any purifn. from whole producer bacteria grown on plates by matrix-assisted laser desorption ionization-time of flight mass spectrometry (MALDI -TOF-MS). When we compared the results of MALDI-TOF-MS performed with samples of whole cells and with samples of crude supernatants of liq. cultures, the former samples led to more efficient bacteriocin detection and required less handling. Nisin and lacticin 481 were both detected from a mixt. of their producer strains, but such a mixt. can yield addnl. signals. We used this method to det. the masses of two lacticin 481 variants, which confirmed at the peptide level the effect of mutations in the corresponding structural gene.

REFERENCE COUNT: 28

L1 ANSWER 5 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:932870 CAPLUS

TITLE: Matrix-assisted laser desorption ionization-time of flight mass spectrometry of lipopeptide biosurfactants in whole cells and culture filtrates of *Bacillus subtilis* C-1 isolated from petroleum sludge

AUTHOR(S): Vater, Joachim; Kablitz, Barbel; Wilde, Christopher; Franke, Peter; Mehta, Neena; Cameotra, Swaranjit Singh

CORPORATE SOURCE: Institut für Chemie, Arbeitsgruppe Biochemie und Molekulare Biologie, Technische Universität Berlin, Berlin, D-10587, Germany

SOURCE: Applied and Environmental Microbiology (2002), 68(12), 6210-6219

CODEN: AEMIDF; ISSN: 0099-2240

PUBLISHER: American Society for Microbiology

DOCUMENT TYPE: Journal

LANGUAGE: English

AB An innovative method was developed for rapid sensitive detection and efficient structural characterization of lipopeptide biosurfactants by matrix-assisted laser desorption ionization-time of flight (MALDI-TOF) mass spectrometry by using whole microbial cells and crude culture filtrates as targets in combination with surface tension measurements. This was done for a bacterial strain that was isolated from petroleum sludge and efficiently produces biosurfactants. This organism was identified by using biochem., physiol., and genetic parameters as a *Bacillus subtilis* strain, designated B. subtilis C-1. This assignment was supported by a mass spectrometric investigation of the secondary metabolite spectrum detd. by whole-cell MALDI-TOF mass spectrometry, which revealed three lipopeptide complexes, the surfactins, the iturins, and the fengycins, which are well-known biosurfactants produced by B. subtilis strains. These compds. were structurally characterized by in situ structure anal. by using postsorce decay MALDI-TOF mass spectrometry. The isoforms were sepd. by miniaturized high-resoln. reversed-phase high-performance liq. chromatog. for mass spectrometric characterization. Iturin compds. which contain unusual fatty acid components were detected.

REFERENCE COUNT: 39

L1 ANSWER 6 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:888151 CAPLUS

TITLE: Preparation of porous n-type silicon sample plates for desorption/ionization on silicon mass spectrometry (DIOS-MS)

AUTHOR(S): Tuomikoski, S.; Huikko, K.; Grigoros, K.; Oestman, P.; Kostianen, R.; Baumann, M.; Abian, J.; Kotiaho, T.; Franssila, S.

CORPORATE SOURCE: Microelectronics Centre, Helsinki University of Technology, HUT, FIN-02015, Finland

SOURCE: Lab on a Chip (2002), 2(4), 247-253

CODEN: LCAHAM; ISSN: 1473-0197

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB This study focuses on porous silicon (pSi) fabrication methods and properties for desorption ionization on silicon mass spectrometry (DIOS-MS). pSi was prepd. using electrochem. etching of n-type silicon in HF-ethanol soln. Porous areas were defined by a double-sided illumination arrangement: front-side porous areas were masked by a stencil mask, eliminating the need for std. photolithog., and backside illumination was used for the backside ohmic contact. Backside illumination improved the uniformity of the porosified areas. Porosification conditions, surface derivatizations and storage conditions were explored to optimize pSi area, pore size and pore depth. Chem. derivatization of the pSi surfaces improved the DIOS-MS performance providing better ionization efficiency and signal stability with lower laser energy. Droplet spreading and drying patterns on pSi were also examd. Pore sizes of 50-200 nm were found to be optimal for droplet evapn. and pore filling with the sample liq., as measured by DIOS efficiency. With DIOS, significantly better detection sensitivity was obtained (e.g. 150 fmol for midazolam) than with desorption ionization from a std. MALDI steel plate without matrix addn. (30 pmol for midazolam). Also the noise that disturbs the detection of low-mol. wt. compds. at  $m/z < 500$  with MALDI could be clearly reduced with DIOS. Low background MS spectra and good detection sensitivity at the 100-150 fmol level for pharmaceutical compds. were achieved with DIOS-MS.

REFERENCE COUNT: 20

L1 ANSWER 7 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:732428 CAPLUS

DOCUMENT NUMBER: 138:75007

TITLE: Matrix-assisted ultraviolet laser-desorption ionization and electrospray-ionization time-of-flight mass spectrometry of sulfated neocarrabiose oligosaccharides

AUTHOR(S): Fukuyama, Yuko; Cancia, Marina; Nonami, Hiroshi; Cerezo, Alberto S.; Erra-Balsells, Rosa; Matulewicz, Maria C.

CORPORATE SOURCE: College of Agriculture, Plant Biophysics/Biochemistry Research Laboratory, Ehime University, Matsuyama, 790-8566, Japan

SOURCE: Carbohydrate Research (2002), 337(17), 1553-1562

CODEN: CRBRAT; ISSN: 0008-6215

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Several com. sulfated neocarrabiose oligosaccharides were analyzed by matrix-assisted UV laser-desorption ionization time-of-flight mass spectrometry (UV-MALDI-TOF-MS). UV-MALDI-TOF-MS was carried out in the linear and reflectron modes and, as routine, in both the pos.- and neg.-ion modes. 2,5-Dihydroxybenzoic acid and nor-harmane were used as matrixes. In the pos.- and neg.-ion modes, with both matrixes, peaks corresponding to  $(M + Na)^+$  and  $(M - Na)^-$  ions, resp., were obtained, with only some signals from glycosidic linkage cleavages (prompt fragmentation). With 2,5-dihydroxybenzoic acid abundant matrix signals were obsd.; nor-harmane afforded very few matrix signals in both ion modes, but more de-sulfation (prompt fragmentation) of the compds. occurred. When the desorption/ionization process was highly efficient, the post-source decay (PSD) fragmentation patterns were also investigated; most of the fragments detected derived from glycosidic linkage cleavages. Electrospray-ionization time-of-flight mass spectrometry (ESI-TOF-MS) in the neg.-ion mode confirmed, with the observation of the  $(M - Na)^-$  and the multiply charged anions, the identity and the purity of the samples.

REFERENCE COUNT: 22

L1 ANSWER 8 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:628033 CAPLUS

DOCUMENT NUMBER: 137:305847

TITLE: "Matrix Addition by Condensation for Matrix-Assisted Laser Desorption/Ionization of Collected Aerosol Particles"

AUTHOR(S): *Jackson, Shelley N.; Murray, Kermit K.*

CORPORATE SOURCE: Department of Chemistry, Louisiana State University, Baton Rouge, LA, 70803, USA

SOURCE: **Analytical Chemistry** (2002), 74(18), 4841-4844

CODEN: ANCHAM; ISSN: 0003-2700

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Condensation of an UV absorbing liq. matrix onto aerosol particles was used to enhance the ionization efficiency of large mols. Lab.-generated particles were coated with matrix, deposited on a sample target, and analyzed by laser desorption mass spectrometry with no other matrix addn. The aerosol was generated in a Collision nebulizer, and the particles were dried in a diffusion dryer before entering a heated region satd. with the liq. matrix 3-nitrobenzyl alc. (NBA) and then entering a cooled condensation region. Matrix-coated particles were collected on a sample target and analyzed using a 337-nm laser and a time-of-flight mass spectrometer. Particles contg. the peptides gramicidin S and gramicidin D were analyzed both with and without the matrix addn. step. Condensation addn. of matrix increased the biomol. ion signal and resulted in mass spectra with less fragmentation and low-mass ion interference.

REFERENCE COUNT: 37

L1 ANSWER 9 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:605920 CAPLUS  
DOCUMENT NUMBER: 137:311596  
TITLE: "Quantitative analysis of technical polymer mixtures by matrix assisted laser desorption/ionization time of flight mass spectrometry"  
AUTHOR(S): *Yan, Wenyan; Gardella, Joseph A.; Wood, Troy D.*  
CORPORATE SOURCE: Bausch and Lomb, Inc., Rochester, NY, USA  
SOURCE: **Journal of the American Society for Mass Spectrometry (2002), 13(8), 914-920**

CODEN: JAMSEF; ISSN: 1044-0305

PUBLISHER: Elsevier Science Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We report quant. MALDI-TOF measurements for poly(dimethylsiloxane) (PDMS) of two different mol. wts. using the relative ratio of the signal intensities of integrated oligomer distributions for these two mol. wt. distributions. By reporting the ratio of intensities of the integrals of two oligomer distributions, we assume that the ionization and desorption efficiencies, crystn. conditions and other factors affecting intensity are similar. Poly(Me methacrylate) (PMMA-33,000) was mixed with PDMS samples to show whether the presence of another material might affect the desorption efficiency. Quant. values for the no.-av. mol. wt. (Mn), wt.-av. mol. wt. (Mw) and polydispersities (D) were calcd. using the oligomer distributions. The results show a linear relationship between the analyte concns. and the signal intensities in the range from 1,000 Da to 10,000 Da, and the desorption efficiency of these two PDMS materials was the same even in the presence of PMMA.

REFERENCE COUNT: 25

L1 ANSWER 10 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:450009 CAPLUS

DOCUMENT NUMBER: 137:17454

TITLE: Isotope-coded ionization-enhancing reagents (ICIER) for high-throughput protein identification and quantitation using matrix-assisted laser desorption ionization mass spectrometry

INVENTOR(S): Qiu, Yongchang; Wang, Jack H.; Hewick, Rodney M.

PATENT ASSIGNEE(S): Genetics Institute, LLC, USA

SOURCE: PCT Int. Appl., 45 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002046770	A2	20020613	WO 2001-US50744	20011022
AU 2002041732	A5	20020618	AU 2002-41732	20011022
US 2003054570	A1	20030320	US 2001-44708	20011022

PRIORITY APPLN. INFO.: US 2000-242645P P 20001023  
WO 2001-US50744 W 20011022

AB The invention concerns arginine-contg. cysteine-modifying compds. useful for MALDI-MS anal. of proteins are provided. These compds. termed isotope-coded ionization enhancement reagents (ICIER) can provide ionization enhancement in MALDI-MS, relative quantitation, and addnl. database searching constraints at the same time without any extra sample manipulation. More specifically, ICIER increase the ionization efficiency of cysteine-contg. peptides by attachment of a guanidino functional group. ICIER also increase the overall hydrophilicity of these peptides due the hydrophilic nature of ICIER and thus increase the percentage of recovery of these peptides during sample handling and processing such as in-gel digestion or liq. chromatog. Finally, a combination of both light and heavy ICIER provides an accurate way to obtain relative quantitation of proteins by MALDI-MIS and addnl. database searching constraints (no. of cysteine residues in every single peptide peak) to increase the confidence of protein identification by peptide mass mapping.

L1 ANSWER 11 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:388061 CAPLUS

DOCUMENT NUMBER: 137:109699

TITLE: "Quantitative Analysis of Copolymers: Influence of the Structure of the Monomer on the Ionization Efficiency in Electrospray Ionization FTMS"

AUTHOR(S): *Koster, Sander; Mulder, Bela; Duursma, Marc C.; Boon, Jaap J.; Philipsen, Harry J. A.; van Velde, Jan W.; Nielen, W. F.; Koster, Chris G.*

CORPORATE SOURCE: Unit for Macromolecular Mass Spectrometry, FOM-Institute for Atomic and Molecular Physics, Amsterdam, 1098 SJ, Neth.

SOURCE: **Macromolecules (2002), 35(13), 4919-4928**

CODEN: MAMOBX; ISSN: 0024-9297

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The influence of the ionization efficiency on the measured copolymer sequence distribution is presented. Large differences in ionization efficiency were obsd. for mixts. of homopolyesters contg. dipropoxylated bisphenol A/adipic acid and dipropoxylated bisphenol A/isophthalic acid and the corresponding copolyester dipropoxylated bisphenol A/isophthalic acid/adipic acid. The adipic acid structure has a higher affinity for the Na cation, which results in more intense peaks for adipic acid contg. oligomers. Relative Na affinities of the oligomers increase with an increasing no. of acid end groups in favor of adipic acid-contg. oligomers. The ESI response of the oligomers depends on the polymer concn. in the sprayed mixt. This makes it impossible to correct for the ionization efficiency necessary for copolymer anal. If differences in ionization efficiency are not cor., the ion intensities in the copolymer mass spectra will show large deviations from the real compn. and no conclusion can be drawn about the chem. (in)homogeneity of the MWD nor the random or block structure of the copolymer. This will also be valid for other cationization techniques like MALDI and FAB.

REFERENCE COUNT: 57

L1 ANSWER 12 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:214548 CAPLUS

DOCUMENT NUMBER: 137:6674

TITLE: Characterization of oligomeric polypropyleneglycol acrylate by GC, SFC and MALDI-TOF-MS

AUTHOR(S): Matsunaga, Morikatsu; Matsushima, Yoshiaki; Yokoi, Hiroaki; Ohtani, Hajime; Tsuge, Shin

CORPORATE SOURCE: Nagoya Reseach & Development Institute, Toagosei Co., Ltd., Nagoya, 455-0027, Japan

SOURCE: Analytical Sciences (2002), 18(3), 277-281

CODEN: ANSCEN; ISSN: 0910-6340

PUBLISHER: Japan Society for Analytical Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Polypropyleneglycol acrylate (PGA), one of the typical acrylic oligomers manufd. industrially, was comprehensively characterized by gas chromatog. (GC), supercrit. fluid chromatog. (SFC) and matrix-assisted laser desorption ionization time-of-flight mass spectrometry (MALDI -TOF-MS). The homologous series of polypropyleneglycol diacrylate (DA), polypropyleneglycol monoacrylate (MA), and unreacted polypropyleneglycol (PG) were obsd. as Na adducts in the MALDI-MS spectra of the PGA samples. The relative intensities of these peaks reflect the distributions of the homologues, although their accurate quantification was generally difficult because of change in the ionization efficiency depending on the chem. structure and the mol. wt. of the species. On the other hand, the DA and the MA homologues were obsd. in the chromatograms obtained by SFC in a temp.-programming mode, while the PG homologues were not detected under the given SFC conditions using UV detection. Here, the detn. of the d.p. of each component in the chromatograms was accomplished through SFC fractionation for the corresponding peaks, followed again by MALDI-TOF-MS measurement. Furthermore, most of the components in the PGA samples were almost completely sepd. in the resulting gas chromatograms, and their unequivocal assignments were made also using the retention data on the gas chromatograms of the SFC fractions. As for the quant. anal., the relative abundances among DA, MA and PG for lower ds.p. can be easily calcd. based on the obsd. gas chromatograms, whereas the distribution of DA and MA can be estd. from the obsd. SFC data even for the relatively higher mol. wt. fractions, which are generally difficult to det. accurately by GC because of their lower volatility. These results demonstrated that even the complex PGA samples were able to be characterized in detail by using GC, SFC and MALDI-TOF-MS complementarily.

REFERENCE COUNT: 17

L1 ANSWER 13 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:164466 CAPLUS

DOCUMENT NUMBER: 136:341256

TITLE: "End-Groups-Dependent MALDI Spectra of Polymer Mixtures"



AUTHOR(S): *Puglisi, Concetto; Samperi, Filippo; Alicata, Rossana; Montaudo, Giorgio*

CORPORATE SOURCE: Istituto per la Chimica e la Tecnologia dei Materiali Polimerici, Consiglio Nazionale delle Ricerche, Catania, 6-95125, Italy

SOURCE: **Macromolecules** (2002), **35**(8), 3000-3007

CODEN: MAMOBX; ISSN: 0024-9297

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB During a work designed to use MALDI-TOF MS to det. the compn. of an equimolar blend of nylon 6 (Ny6) and poly(butylene terephthalate) (PBT), the MALDI-TOF mass spectrum showed a surprising strong imbalance between the two components. The predominance of Ny6 oligomers over the PBT oligomers terminated with hydroxyl end chains is signaled by the appearance of specific peaks in the MALDI-TOF mass spectra. Since the av. molar mass and the polydispersion of the two polymers are comparable, the MALDI-TOF MS ionization efficiency is quite different for the two components of the blend. This finding prompted us to a more detailed study, and to synthesize a no. of Ny6 and PBT samples terminated with different end groups, to analyze their equimolar blends by MALDI-TOF MS. The results reported in the present study may help clarifying some fundamental aspects about the mechanisms of ions formation, when MALDI-TOF mass spectrometry is applied to macromols. End groups ionization efficiency appears to be the most important parameter in detg. the relative intensity of peaks in the MALDI-TOF mass spectra of the polymer blends studied. End-groups-dependent ionization of MALDI-TOF mass species is the key to rationalize the relative peak intensity in MALDI-TOF mass spectra of polymer mixts. Understanding of ionization efficiency mechanisms is essential to the quant. applications of MALDI-TOF MS.

REFERENCE COUNT: 21

L1 ANSWER 14 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:124106 CAPLUS

DOCUMENT NUMBER: 136:341398

TITLE: Influence of chain end groups on the matrix-assisted laser desorption/ionization spectra of polymer blends

AUTHOR(S): Alicata, R.; Montaudo, G.; Puglisi, C.; Samperi, F.

CORPORATE SOURCE: Dipartimento di Scienze Chimiche, Universita di Catania, Catania, 95125, Italy

SOURCE: *Rapid Communications in Mass Spectrometry* (2002), **16**(4), 248-260

CODEN: RCMSEF; ISSN: 0951-4198

PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The pos. ion matrix-assisted laser desorption/ionization (MALDI) spectrum of an equimolar blend of Nylon 6 (NY 6) and hydroxyl-terminated polybutylene terephthalate (PBT) shows a surprisingly strong imbalance between the two components. Since the av. molar masses and the polydispersion of the two polymers are comparable, it follows that the efficiency of MALDI is quite different for the two components of the blend.

This finding prompted us to a more detailed study, and to synthesize NY and PBT samples terminated with different end groups, in order to analyze their blends by MALDI. The neg. ion MALDI spectra of the mixts. investigated show that PBT samples do not yield signals, so that only NY peaks appear in these spectra. By comparing pos. and neg. ion MALDI spectra of mixts. of NY terminated with various end groups, it was found that the peak intensity depends on the nature of the end groups. The results reported in the present study may help to clarify some fundamental aspects of the mechanisms of ion formation, when MALDI mass spectrometry is applied to macromols. End group ionization efficiency appears to be the most important parameter in detg. the relative intensity of peaks in the MALDI spectra of the polymer blends investigated. End-group-dependent ionization is the key to the rationalization of the relative peak intensities in MALDI spectra of polymer mixts.

REFERENCE COUNT: 19 IN THE RE FORMAT

L1 ANSWER 15 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:740368 CAPLUS

DOCUMENT NUMBER: 135:354891

TITLE: Capillary electrophoresis using a surfactant-treated capillary coupled with offline matrix-assisted laser desorption ionization mass spectrometry for high efficiency and sensitivity detection of proteins

AUTHOR(S): Yeung, K. K.-C.; Kiceniuk, A. G.; Li, L.

CORPORATE SOURCE: Faculty of Science, Department of Chemistry, University of Alberta, Edmonton, AB, T6G 2G2, Can.

SOURCE: Journal of Chromatography, A (2001), 931(1-2), 153-162

CODEN: JCRAEY; ISSN: 0021-9673

PUBLISHER: Elsevier Science B. V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A method of combining capillary electrophoresis (CE) using a surfactant-modified capillary with matrix-assisted laser desorption ionization (MALDI) mass spectrometry (MS) is described for protein anal. The CE-MALDI-MS coupling is based on CE fraction collection of nanoliter vol. samples in less than 5  $\mu$ l of dil. acid. This offline coupling does not require any special instrumentation and can be readily performed with com. instruments. Protein adsorption during CE sepn. is prevented by coating the capillary with the surfactant didodecyldimethylammonium bromide. This surfactant binds strongly with the capillary wall, hence it does not desorb significantly to interfere with subsequent MALDI-MS anal. It is shown that the use of a dil. acid for CE fraction collection is advantageous in lowering the detection limit of MALDI-MS compared to using an electrophoretic buffer. The detection limit for proteins such as cytochrome c is 23 fmol injected for CE, or 1.2 fmol spotted for MALDI-MS. This sensitivity is comparable to alternative CE-MALDI-MS coupling techniques using direct CE sample deposition on the MALDI target. In addn., the fraction collection approach has the advantage of allowing multiple reactions to be carried out on the fractionated sample. These reactions are very important in protein identification and structure anal.

REFERENCE COUNT: 30

L1 ANSWER 16 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:633942 CAPLUS

DOCUMENT NUMBER: 135:282354

TITLE: Two-photon ionization thresholds of matrix-assisted laser desorption/ionization matrix clusters

AUTHOR(S): Lin, Qiong; Knochenmuss, Richard

CORPORATE SOURCE: Laboratorium für Organische Chemie, Swiss Federal Institute of Technology Zurich, Zurich, CH-8092, Switz.

SOURCE: Rapid Communications in Mass Spectrometry (2001), 15(16), 1422-1426

CODEN: RCMSEF; ISSN: 0951-4198

PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Direct two-photon ionization of the matrix was considered a likely primary ionization mechanism in matrix-assisted laser desorption/ionization (MALDI) mass spectrometry. This mechanism requires that the vertical ionization threshold of matrix materials be below twice the laser photon energy. Because dimers and larger aggregates may be numerous in the early stages of the MALDI plume expansion, their ionization thresholds are important as well. Two-color two-photon ionization was used to det. the ionization thresholds of jet cooled clusters of an important matrix, 2,5-dihydroxy benzoic acid (DHB), and mixed clusters with the thermal decompn. product of DHB, hydroquinone. The thresholds of the clusters were reduced by only a few tenths of an eV compared to the monomers, to an apparent limit of 7.82 eV for pure DHB clusters. None of the studied clusters can be directly ionized by two nitrogen laser photons (7.36 eV), and the ionization efficiency at the thresholds is low.

REFERENCE COUNT: 18

L1 ANSWER 17 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:609582 CAPLUS

DOCUMENT NUMBER: 136:144373

TITLE: "Detection of 25,000 molecules of substance P by MALDI-TOF mass spectrometry and investigations into the fundamental limits of detection in MALDI"

AUTHOR(S): Keller, B. O.; Li, L.

CORPORATE SOURCE: Department of Chemistry, University of Alberta, Edmonton, AB, Can.

SOURCE: Journal of the American Society for Mass Spectrometry (2001), 12(9), 1055-1063

CODEN: JAMSEF; ISSN: 1044-0305

PUBLISHER: Elsevier Science Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Mass spectrometric anal. of peptides with a total sample loading of several tens of thousands of mols. (i.e., low zeptomoles) is demonstrated. At this low level of sample loading, it becomes important to consider several very unique tech. and fundamental aspects that are not obvious in compatible expts. with a higher amt. of sample loading. Prudent matrix prepn. allows anal. of peptides from solns. with picomolar concns. in

matrix-assisted laser desorption ionization (MALDI) mass spectrometry. Using microspot MALDI the authors demonstrate the introduction and detection of 25,000 mols. of Substance P in a time-of-flight mass spectrometer. A method based on probability theory is presented to est. the min. no. of ions required for generating a statistically significant isotope peak pattern of peptide ions. The low boundary of ionization efficiency is 1-2% for Substance P. In addn., comparison of macro- and microspot sample deposition techniques for Substance P shows that under the exptl. conditions used, a min. of .apprx.5 analyte mols. per .mu.m2 are necessary to generate useful signals. Implications of these results on further mass spectrometric developments towards even more sensitive detection are discussed.

REFERENCE COUNT: 30

L1 ANSWER 18 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:533021 CAPLUS

DOCUMENT NUMBER: 136:161899

TITLE: Rapid characterization of DNA oligomers and genotyping of single nucleotide polymorphism using nucleotide-specific mass tags

AUTHOR(S): Abdi, Fadi; Bradbury, E. Morton; Doggett, Norman; Chen, Xian

CORPORATE SOURCE: C-ACS, Chemistry Division, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM, 87544, USA

SOURCE: Nucleic Acids Research (2001), 29(13), e61/1-e61/11

CODEN: NARHAD; ISSN: 0305-1048

PUBLISHER: Oxford University Press

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Using currently available MS-based methods, accurate mass measurements are essential for the characterization of DNA oligomers. However, there is a lack of specificity in mass peaks when the characterization of individual DNA species in a mass spectrum is dependent solely upon the mass-to-charge ratio ( $m/z$ ). Here, we utilize nucleotide-specific tagging with stable isotopes to provide internal signatures that quant. display the nucleotide content of oligomer peaks in MS spectra. The characteristic mass-split patterns induced by the partially  $^{13}\text{C}/^{15}\text{N}$ -enriched dNTPs in DNA oligomers indicate the no. of labeled precursors and in turn the base substitution in each mass peak, and provide for efficient SNP detection. Signals in mass spectra not only reflect the masses of particular DNA oligomers, but also their specific compn. of particular nucleotides. The measurements of mass tags are relative in the mass-split pattern and, hence, the accuracy of the detn. of nucleotide substitution is indirectly increased. For high sample throughput,  $^{13}\text{C}/^{15}\text{N}$ -labeled sequences of interest have been generated, excised in soln. and purified for MS anal. in a single-tube format. This method can substantially improve the specificity, accuracy and efficiency of mass spectrometry in the characterization of DNA oligomers and genetic variations.

REFERENCE COUNT: 5

L1 ANSWER 19 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:456210 CAPLUS

DOCUMENT NUMBER: 135:73604

TITLE: Effect of strong detergents and chaotropes on the detection of proteins in two-dimensional gels

AUTHOR(S): Fountoulakis, Michael; Takacs, Bela

CORPORATE SOURCE: Genomics Technologies, Pharmaceutical Research, F. Hoffmann-La Roche, Basel, 4070, Switz.

SOURCE: Electrophoresis (2001), 22(9), 1593-1602

CODEN: ELCTDN; ISSN: 0173-0835

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The solubilization of a particular protein is mandatory for its subsequent resoln. and detection in two-dimensional gels. However, the extn. solns., that are compatible with the first-dimensional sepn. step, such as urea and 3-[(3-cholamidopropyl)dimethylammonio]-1-propanesulfonate (CHAPS), do not solubilize all proteins in a sample. We studied the effect of various common, strong detergents and chaotropes, widely used as solubilizing agents, such as SDS, lithium dodecyl sulfate and guanidine hydrochloride, on the solubilization of the total and membrane proteins of the bacterium *Haemophilus influenzae*. The proteins solubilized with each system were analyzed by two-dimensional electrophoresis and these of interest were identified by matrix assisted laser desorption/ionization-mass spectrometry (MALDI-MS). Use of SDS, lithium dodecyl sulfate or guanidine hydrochloride for the solubilization of total proteins of the micro-organism resulted in the detection of several addnl. spots, representing mainly outer membrane proteins, in comparison with those detected in the sol. protein fraction. Solubilization of the proteins of the cell envelope fraction with SDS did not result in a more efficient protein detection when compared to the extn. with the urea/CHAPS system. When the dry immobilized pH gradient strips were rehydrated in a soln. contg. the proteins of the membrane fraction solubilized with SDS or lithium dodecyl sulfate, a larger no. of protein spots were detected in comparison with strips that were rehydrated in the urea/CHAPS soln. However, no improvement was obsd. in comparison with protein application in sample cups. The addnl. proteins detected with the use of strong detergents and chaotropes are in the majority difficult to solubilize and less hydrophobic proteins.

REFERENCE COUNT: 45

L1 ANSWER 20 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:105309 CAPLUS

DOCUMENT NUMBER: 134:219101

TITLE: "Single molecule detector for mass spectrometry with mass independent detection efficiency"

AUTHOR(S): *Twerenbold, Damian; Gerber, Daniel; Gritti, Dominique; Gonin, Yvan; Netuschill, Alexandre; Rossel, Frederic; Schenker, Dominique; Vuilleumier, Jean-Luc*

CORPORATE SOURCE: Institut de Physique, Universite Neuchatel, Neuchatel, CH-2000, Switz.

SOURCE: *Proteomics* (2001), 1(1), 66-69

Published in: *Electrophoresis*, 22(2)

CODEN: PROTC7; ISSN: 1615-9853

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Exptl. results from equimolar PEG and protein stds. samples are presented from a MALDI-TOF mass spectrometer equipped with both ionizing detectors and the novel single mol. sensitive cryodetectors. The data are consistent with a model hypothesis suggesting that the obsd. decrease in signal strength in conventional ionizing detector MALDI-TOF mass spectrometers can be explained by the exponentially decreasing quantum efficiency of ionizing detectors. Cryodetectors, in contrast, have a mass independent detection efficiency of 100% on impact and provide addnl. information on the mol. state owing to the calorimetric nature of the detection mechanism.

REFERENCE COUNT: 13

L1 ANSWER 21 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2000:253487 CAPLUS

DOCUMENT NUMBER: 132:354515

TITLE: Aluminium junctions as macromolecule detectors and comparison with ionizing detectors

AUTHOR(S): Gervasio, G.; Gerber, D.; Gritti, D.; Gonin, Y.; Twerenbold, D.; Vuilleumier, J.-L.

CORPORATE SOURCE: IPH -Institute de Physique de l'Universite de Neuchatel, Neuchatel, 2000, Switz.

SOURCE: Nuclear Instruments & Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors, and Associated Equipment (2000), 444(1-2), 389-394

CODEN: NIMAER; ISSN: 0168-9002

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Cryogenic particle detectors were proposed as alternative detectors for heavy mol. mass spectrometry (T., 1996). The concept was demonstrated by various groups in the last 3 yrs. The single-mol. detection efficiency is independent of mass and close to the geometrical beam coverage. The charged state of the macromol. can be detd. by the pulse height of the cryodetector signal (G. Hilton, 1998). The authors present results from Al junctions (50 .mu.m.times.400 .mu.m) cooled by a diln. refrigerator. The Al-junction detectors were exposed to 6 keV x-rays from a <sup>55</sup>Fe source and to a variety of macromols., including IgG and polyethylene-glycols (PEGs). Identical samples were measured with a conventional secondary electron multiplier detector, allowing a sensitivity comparison. Data, combined with measurements from other groups, suggest that the MALDI extn. does not affect too much the sample mass distribution, and that secondary electron detector sensitivity decreases with decreasing mol. velocity as  $\exp(-(v/v_0)^{3.5})$  with  $v_0$  being of the order of 50 km/s.

REFERENCE COUNT: 11

L1 ANSWER 22 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1999:725599 CAPLUS

DOCUMENT NUMBER: 132:134234

TITLE: "Matrix influence on the formation of positively charged oligonucleotides in matrix-assisted laser desorption/ionization mass spectrometry"

AUTHOR(S): *Chou, Chau-Wen; Williams, Peter; Limbach, Patrick A.*

CORPORATE SOURCE: Department of Chemistry, Louisiana State University,  
Baton Rouge, LA, 70803, USA

SOURCE: **International Journal of Mass Spectrometry (1999), 193(1), 15-27**

CODEN: IMSPF8; ISSN: 1387-3806

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The ionization efficiency of various UV

matrix-assisted laser desorption/ionization mass spectrometry (MALDI-MS) matrixes was investigated. A site of fixed pos. charge was generated on an oligonucleotide by addn. of a quaternary ammonium. This quaternary ammonium-tagged oligonucleotide was then used as an internal std. to probe the relative ionization capabilities of 3-hydroxypicolinic acid (3-HPA), 2',4',6'-trihydroxyacetophenone (THAP) and 2,5-dihydroxybenzoic acid (DHBA) in pos.-ion mode. MALDI-MS anal. of equimolar mixts. of the quaternary ammonium-tagged oligonucleotide and an unmodified polythymidylic acid, dT12, found that 3-HPA yielded more abundant protonated dT12 mol. ions than either THAP or DHBA. These results demonstrate that the low ion yields previously reported for polythymidylic acid are due to the matrix utilized and are not due to the low proton affinity of thymidine. Primary, secondary and tertiary amines were also incorporated into dT12 to examine the effect of these different amines on the protonation efficiency of the three matrixes under investigation. Similar results were obtained, regardless of the amine-tag utilized, with protonation efficiency following the trend 3-HPA > THAP > DHBA. Consideration of the various factors that might influence the overall prodn. of pos. charged polythymidylic acid finds that it is the matrix: phosphodiester backbone interaction that might play the important role in detg. the optimal MALDI-MS response. These results are a step towards understanding the matrix properties necessary for optimal prodn. of oligonucleotide mol. ions in MALDI-MS.

REFERENCE COUNT: 47

L1 ANSWER 23 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1999:682127 CAPLUS

DOCUMENT NUMBER: 132:47097

TITLE: Polyamine co-matrices for matrix-assisted laser desorption/ionization mass spectrometry of oligonucleotides

AUTHOR(S): Vandell, Victor E.; Limbach, Patrick A.

CORPORATE SOURCE: Department of Chemistry, Louisiana State University,  
Baton Rouge, LA, 70803, USA

SOURCE: **Rapid Communications in Mass Spectrometry (1999), 13(20), 2014-2021**

CODEN: RCMSEF; ISSN: 0951-4198

PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The anal. of oligonucleotides using matrix-assisted laser desorption/ionization mass spectrometry (MALDI-MS) has led to the investigation of the use of matrix additives (i.e., co-matrixes) to help improve the poor spectral quality commonly obsd. during the anal. of this class of compds. The use of certain matrix additives in MALDI-MS has been investigated previously, and these additives have been shown to enhance the desorption/ionization efficiency of oligonucleotides during the MALDI expt. Specifically, amine bases, such as piperidine, imidazole, and triethylamine, have been shown to improve mass spectral quality as assessed by improved mol. ion resoln. and increased mol. ion abundance. These improvements occur due to competition between the oligonucleotide and the co-matrix for protons generated during the MALDI event. Co-matrixes with proton affinities near or above the proton affinities of the nucleotide residues serve as proton sinks during the desorption/ionization process. In this work, we have investigated the use of polyamines as co-matrixes for MALDI mass spectrometric anal. of oligonucleotides. Spermine tetrahydrochloride, spermine, spermidine trihydrochloride, and spermidine were evaluated for their effectiveness at enhancing the mass spectral quality of oligonucleotides analyzed using MALDI-MS. The soln.-phase pKb values and the gas-phase proton affinities of these polyamines were detd., and it was found that the polyamines appear to be more basic than the monofunctional amines investigated previously. The mass spectral data shows that spermidine and spermine are extremely effective co-matrixes, yielding improved mol. ion resoln. and mol. ion abundances. The spermine co-matrixes are more effective than the spermidine co-matrixes, but adduction problems with the spermine co-matrixes limits their overall utility. In general, polyamine co-matrixes are found to be more effective than monofunctional amine co-matrixes at improving the mass spectral data obtained during MALDI-MS of oligonucleotides.

REFERENCE COUNT: 32

L1 ANSWER 24 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1999:455952 CAPLUS

DOCUMENT NUMBER: 131:225649

TITLE: "Studies of peptide binding to allyl amine and vinyl acetic acid-modified polymers using matrix-assisted laser desorption/ionization mass spectrometry"

AUTHOR(S): *Walker, Angela K.; Qiu, Haibo; Wu, Yuliang; Timmons, Richard B.; Kinsel, Gary R.*

CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Texas at Arlington, Arlington, TX, 76019-0065, USA

SOURCE: **Analytical Biochemistry (1999), 271(2), 123-130**

CODEN: ANBCA2; ISSN: 0003-2697

PUBLISHER: Academic Press

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Previous studies have shown that increases in surface-peptide binding affinity result in decreases in peptide matrix-assisted laser desorption/ionization (MALDI) mass spectrometry (MS) ion signals. The present work demonstrates that, with appropriate corrections for peptide ionization efficiency under MALDI conditions, relative surface-peptide binding affinities can be assayed using the MALDI MS methodol. Peptides with



a range of pI values are allowed to interact with amine-modified and carboxylic acid-modified polymer surfaces (produced by pulsed radiofrequency plasma polymn. of allyl amine and vinyl acetic acid) in buffered solns. of neutral pH. Because of the net pos. and neg. charges assocd. with the peptides and surfaces in soln., both electrostatic and hydrophilic interactions play a role in the surface-peptide interaction. Consistent with expectations, the peptide MALDI ion signals for peptides with net neg. charges in soln. are smaller than those for peptides with net pos. charges in soln. when the peptides are allowed to interact with pos. charged surfaces. A reversal of the relative peptide MALDI ion signal intensities is obsd. when the same peptides are allowed to interact with neg. charged surfaces. Cumulatively, the results demonstrate that even modest changes in surface-peptide interactions can be comparatively probed by MALDI mass spectrometry. (c) 1999 Academic Press.

REFERENCE COUNT: 29

L1 ANSWER 25 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1999:233429 CAPLUS

DOCUMENT NUMBER: 131:65300

TITLE: Gas-phase oxidation and reduction of some 1-(2-benzothiazolyl)-3,5-diphenyl formazans. Complex formation with transition metals under laser desorption ionization

AUTHOR(S): Nuutinen, Jari M. J.; Romppanen, Ritva; Makinen, Silja; Vainiotalo, Pirjo

CORPORATE SOURCE: Department of Chemistry, University of Joensuu, Joensuu, FIN-80101, Finland

SOURCE: Journal of the American Society for Mass Spectrometry (1999), 10(4), 339-346

CODEN: JAMSEF; ISSN: 1044-0305

PUBLISHER: Elsevier Science Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Five differently substituted 1-(2-benzothiazolyl)-3,5-diphenyl formazans were studied by laser desorption ionization (LDI) and matrix assisted laser desorption/ionization (MALDI) mass spectrometry. The best explanation of the results is that the formazan mols. are photoionized to mol. radical ions, which then further react by ion-mol. reactions. Supporting this proposal was the abundant formation of  $[M - H]^+$  ions under LDI. These ions are not obsd. at all under either electron or chem. ionization. Under MALDI, the extent of the oxidn. process is clearly dependent on the ability of the matrix to act as a reducing agent. With transition metals the formazans formed singly charged 1:2 metal:formazan complexes. The most stable electronic configuration of the complex detd. the oxidn. state of the metal regardless of its initial oxidn. state. In some cases, this process also demanded a gas-phase redn. of the formazan. The ionization efficiency and affinity for complex formation depended on the substituent at the 3-Ph group; both were increased by an electron donating substituent. The formazans were also tested as potential matrixes for MALDI. Reasonable results were obsd. for several groups of compds.; however, only the piperazine ligands produced higher quality spectra with formazans than with common com. matrixes.

REFERENCE COUNT: 37

L1 ANSWER 26 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1998:677461 CAPLUS

DOCUMENT NUMBER: 130:38881

TITLE: High-performance liquid chromatography of polyethylene glycols as their .alpha.,.omega.-bis(1-naphthylurethane) derivatives and signal monitoring by fluorescence detection

AUTHOR(S): Rissler, Klaus; Wyttenbach, Nicole; Bornsen, K. Olaf

CORPORATE SOURCE: Performance Polymers, Ciba Specialty Chemicals Inc., Basel, CH-4002, Switz.

SOURCE: Journal of Chromatography, A (1998), 822(2), 189-206

CODEN: JCRAEY; ISSN: 0021-9673

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Polyethylene glycols (PEGs) of av. mol. mass (Mr) 600, 1000 and 3000 were converted to their .alpha.,.omega.-bis(1-naphthylurethane) derivs. with 1-naphthyl-isocyanate and subjected to high-performance liq. chromatog. on a Si 80 bare silica gel stationary phase. Signal monitoring was done by fluorescence detection at wavelengths of 232 nm for excitation and 358 nm for emission. A binary acetonitrile-water gradient effected good sepn. of PEG 600 and PEG 1000 into a wide variety of individual oligomers and almost baseline sepn. was achieved for PEG 600 and PEG 1000. In contrast, PEG 3000 requires a ternary acetonitrile-water-THF gradient for both efficient elution and acceptable satisfactory signal resohn. Although sepn. of PEG 3000 into individual oligomers was substantially lower than that obsd. for PEG 600 and PEG 1000, the chromatograms impressively reveal the oligomeric compn. of the polyether sample. Using serial dilns. of the .alpha.,.omega.-bis(1-naphthylurethane) derivs., the detection limits for PEG 600, PEG 1000 and PEG 3000 are approx. 0.1 ppm, resp. Using 50 .mu.l of sample dissolved in either water or physiol. saline, a detection limit of 1 .mu.g/mL was achieved corresponding to an abs. amt. injected of 10 ng. Considering both sepn. efficiency and detection sensitivity, this new technique, termed as a pseudo-reversed-phase sepn. process, may therefore be applicable to investigations of intestinal permeability and resorption in the living organism. Furthermore, with PEG 3000 as model compd., incorporation of 2 1-naphthyl substituents to the corresponding .alpha.,.omega.-bis(1-naphthylurethane) deriv. was confirmed by matrix assisted laser desorption ionization time-of-flight mass spectrometry (MALDI-TOF-MS).

REFERENCE COUNT: 42

L1 ANSWER 27 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1998:468401 CAPLUS

DOCUMENT NUMBER: 129:185860

TITLE: Nonradioactive phosphopeptide assay by matrix-assisted laser desorption ionization time-of-flight mass spectrometry: application to calcium/calmodulin-dependent protein kinase II

AUTHOR(S): Matsumoto, Hiroyuki; Kahn, Esther S.; Komori, Naoka

CORPORATE SOURCE: Department of Biochemistry and Molecular Biology, University of Oklahoma Health Sciences Center, Oklahoma City, OK, 73190, USA

SOURCE: Analytical Biochemistry (1998), 260(2), 188-194

CODEN: ANBCA2; ISSN: 0003-2697

PUBLISHER: Academic Press

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Matrix-assisted laser desorption ionization time-of-flight mass spectrometry (MALDI-TOF) was used to quantify the phosphopeptide produced by calcium/calmodulin-dependent protein kinase II (CaMK II). MALDI-TOF measurements were performed in a linear and pos. ion mode with delayed extn. excited at various laser powers and at different sampling positions, i.e., different loci of laser illumination. The authors find that the ratio of the peak area of the substrate (S) to that of its monophosphorylated form (SP) for a given mixt. is const., independent of the laser powers and/or of the sample loci illuminated by the laser. The authors also find that the fraction of phosphorylation detd. by MALDI-TOF, or fMALDI-TOF, is proportionally smaller than that detd. by HPLC, or fHPLC; the ratio fMALDI-TOF/fHPLC was  $0.797 \pm 0.0229$  (99% confidence limit,  $n = 7$ ) for a 30-mer peptide substrate used in this study. A low mass gate, which turns off the detector temporarily, improved the ratio fMALDI-TOF/fHPLC  $0.917 \pm 0.0184$  (99% confidence limit,  $n = 7$ ). Our interpretation of this result is that the redn. of the phosphopeptide peak in the MALDI-TOF measurement is likely to be caused by a temporal loss of detector function rather than by a lower efficiency of ionization for the phosphopeptide compared with its parent species. In these measurements the exptl. errors, up to the 50% phosphorylation state, were less than 5%. After an adjustment made based on the fMALDI-TOF/fHPLC ratio of 0.917, MALDI-TOF gave an accurate measurement for the kinetics of the CaMK II phosphorylation reaction. Since only a small vol. of the reaction mixt., typically contg. 3 to 50 pmol of substrate, is required for the MALDI-TOF measurement, this method can be adapted to a nonradioactive microscale assay for CaMK II and also for other protein kinases. (c) 1998 Academic Press.

REFERENCE COUNT: 15

L1 ANSWER 28 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1998:380685 CAPLUS

DOCUMENT NUMBER: 129:158825

TITLE: Characterization of carbohydrates using a combination of derivatization, high-performance liquid chromatography and mass spectrometry

AUTHOR(S): Shen, Xiaodong; Perreault, Helene

CORPORATE SOURCE: Department of Chemistry, University of Manitoba, 144 Dysart Road, Winnipeg, MB, R3T 2N2, Can.

SOURCE: Journal of Chromatography, A (1998), 811(1 + 2), 47-59

CODEN: JCRAEY; ISSN: 0021-9673

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A combination of derivatization methods, chromatog. techniques and mass spectrometric ionization modes have been explored for the characterization of small sugars and medium-size oligosaccharides. Derivatization using 1-phenyl-3-methyl-5-

pyrazolone (PMP) was preferred over pyridylation (PA) owing to the simplicity of the reaction method, and also to enhanced ionization efficiency of the PMP derivs. relative to aminopyridyl sugars. The good quality and ease of sepn. of PMP derivs. by high-performance liq. chromatog. were also advantages of using PMP derivatization rather than pyridylation. PMP- and PA-monosaccharides produced abundant ions by either fast atom bombardment (FAB), electrospray ionization (ESI) or matrix-assisted laser desorption/ionization (MALDI). The PA and PMP derivs. of lactose, fucosyllactose and sialyllactose yielded FAB spectra with low S/N ratios, whereas ESI and MALDI produced better spectra with a hundredth of the material used for FAB. In general, PMP derivs. of these di- and trisaccharides gave rise to stronger signals than PA analogs. For oligosaccharides contg. more than three sugar rings, only PMP was used for derivatization, FAB was dropped and only ESI and MALDI were utilized.

REFERENCE COUNT: 35

L1 ANSWER 29 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1997:380926 CAPLUS

DOCUMENT NUMBER: 127:34758

TITLE: "Characterization of Polyesters by Matrix-Assisted Laser Desorption Ionization Mass Spectrometry"

AUTHOR(S): *Williams, John B.; Gusev, Arkady I.; Hercules, David M.*

CORPORATE SOURCE: Department of Chemistry, University of Pittsburgh,  
Pittsburgh, PA, 15260, USA

SOURCE: **Macromolecules (1997), 30(13), 3781-3787**

CODEN: MAMOBX; ISSN: 0024-9297

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of aliph. polyesters, characterized by asym. oligomer distributions, heteroterminated linear chains, and cyclic oligomers, were studied using MALDI. The results from structural characterization of these materials was compared with those acquired using fast atom bombardment mass spectrometry, electrospray ionization mass spectrometry (ESI-MS), NMR spectroscopy, and end group titrn. Information on the compn. of these polymers obtained from MALDI, ESI-MS, and end group titrn. showed reasonable agreement. However, the MALDI ionization efficiency appeared to be higher for carboxyl-terminated oligomers. MALDI mol. wt. detn. were contrasted with those from GPC and NMR. Reasons for disparities in the results between the 3 methods are discussed. The feasibility of using acidolysis for structural characterization of high mol. wt. or insol. materials was explored. Reaction of the polyesters with trifluoroacetic acid produced mono- and bis(trifluoroacetate) esters of the starting material. The products were characterized and the progress of the reaction was monitored using MALDI.

L1 ANSWER 30 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1997:313507 CAPLUS

DOCUMENT NUMBER: 126:302502

TITLE: Mass spectrometric structure determination of spider toxins: arginine-containing acylpolyamines from venoms of Brazilian garden spider *Nephilengys cruentata*

AUTHOR(S): Palma, Mario Sergio; Itagaki, Yasuhiro; Fujita, Tsuyoshi; Hisada, Miki; Naoki, Hideo; Nakajima, Terumi

CORPORATE SOURCE: Laboratory of Molecular Biology, Institute of Biosciences/CEVAP, University of Sao Paulo State (UNESP), Sao Paulo, Brazil

SOURCE: *Natural Toxins* (1997), 5(2), 47-57

CODEN: NATOEE; ISSN: 1056-9014

PUBLISHER: Wiley-Liss

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new strategy to characterize glutaminergic blocker acylpolyamines stored in a spider venom with mass spectrometry is described. The crude spider venom exts. are amenable to direct MALDI mass spectrometry anal. which provides a rapid and accurate means of measuring the mol. wts. of acylpolyamines without the isolation of individual samples. Compared with the previously developed  $\mu$ -column HPLC/MS method, this procedure provides more efficient detection and identification of complex venom constituents. Twenty-five acylpolyamines were detected from Brazilian garden spider *Nephilengys cruentata* crude venom exts. by both HPLC/MS and MALDI-mass spectrometry. These acylpolyamine structures were detd. by high-energy collision induced dissocn. MS/MS method. Most of the compds. were classified into the previously reported generalized structures types A to D, which were found from the venom of *Nephilengys borbonica*. The structures of four acylpolyamines (M + H)<sup>+</sup>, m/z 623, 646, 688, and 745, which were not contained in the venom of *Nephilengys borbonica* were detd. to have arginine at the polyamine chain terminal and were named NPTX-622, -645, -687, and -744, resp.

L1 ANSWER 31 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1997:109668 CAPLUS

DOCUMENT NUMBER: 126:222454

TITLE: "Analysis of DNA by "charge tagging" and matrix-assisted laser desorption/ionization mass spectrometry"

AUTHOR(S): Gut, Ivo G.; Jeffery, William A.; Pappin, Darryl J. C.; Beck, Stephan

CORPORATE SOURCE: DNA Sequencing Laboratory, Imperial Cancer Research Fund, London, WC2A 3PX, UK

SOURCE: *Rapid Communications in Mass Spectrometry* (1997), 11(1), 43-50

CODEN: RCMSEF; ISSN: 0951-4198

PUBLISHER: Wiley

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We have developed a method to quant. attach quaternary ammonium fixed charge tags to the 5' or 3'NH<sub>2</sub> ends of DNA using N-hydroxysuccinimidyl ester chem. The chem. conditions for tagging were chosen so that tagging takes place exclusively on aliph. NH<sub>2</sub> groups while base amino groups remain unmodified. The charge tagging chem. was combined with a previously developed backbone alkylation procedure for phosphorothioate DNA. The efficiency of the detection in matrix-assisted laser desorption/ionization (MALDI) mass spectrometry of unmodified and modified DNA (phosphorothioate backbone, charge tagged, backbone alkylated, and charge tagged and

backbone alkylated) was investigated using a series of different matrixes. For .alpha.-cyano-4-hydroxycinnamic acid (a matrix, commonly used for the anal. of proteins, but which gives unsatisfactory results with unmodified DNA). For instance, the charge tagged and backbone alkylated DNA is detectable with a sensitivity and resolu. comparable with that for peptides. The combination of charge tagging and backbone alkylation with the use of a suitable matrix improves the detectability of small oligonucleotides by MALDI by a factor greater than 100 compared to unmodified oligonucleotides.

L1 ANSWER 32 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1997:43537 CAPLUS

DOCUMENT NUMBER: 126:168617

TITLE: "High-efficiency detection of 66,000-Da protein molecules using a cryogenic detector in a matrix-assisted laser desorption/ionization [MALDI] time-of-flight mass spectrometer"

AUTHOR(S): *Frank, M.; Mears, C. A.; Labov, Simon E.; Benner, W. H.; Horn, D.; Jaklevic, J. M.; Barfknecht, A. T.*

CORPORATE SOURCE: Physics Space Technol., Lawrence Livermore Natl. Lab., Livermore, CA, 94551, USA

SOURCE: **Rapid Communications in Mass Spectrometry (1996), 10(15), 1946-1950**

CODEN: RCMSEF; ISSN: 0951-4198

PUBLISHER: Wiley

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We present the first exptl. results obtained using a cryogenically-cooled Nb-Al<sub>2</sub>O<sub>3</sub>-Nb superconductor-insulator-superconductor (SIS) tunnel junction detector operating at 1.3 K as an ion detector in a time-of-flight mass spectrometer. As opposed to microchannel-plate ion detectors (MCPs) commonly used in such systems, cryogenic detectors such as SIS detectors offer a near 100% detection efficiency for all ions including single, very massive, slow-moving macromols. We describe the operating principle of a SIS detector and its use as an ion detector in our MALDI time-of-flight mass spectrometer and compare its response to an MCP detector operated in the same system. To our knowledge, this is the first direct comparison of these detector types in this application. A comparison of count rates and time-of-flight spectra obtained with both detectors for human serum albumin (mol. wt. 66,000 Da) indicates a 2-3 orders of magnitude higher detection efficiency per unit area for the SIS detector at this mass. For higher mol. masses we expect an even higher relative efficiency for cryogenic detectors since MCPs show a rapid decline in detection efficiency as ion mass increases, which is not expected to be the case for cryogenic detectors. Our results imply that time-of-flight techniques could be extended beyond the current upper mass limit if cryogenic detectors are used. Initially, cryogenic detectors will be used for the anal. of large protein mols. If non-fragmenting ionization techniques can be perfected, cryogenic detectors will also open the possibility of the rapid anal. of large DNA mols. and perhaps intact microorganisms.

L1 ANSWER 33 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1996:630505 CAPLUS  
DOCUMENT NUMBER: 125:269852  
TITLE: Analysis by mass spectrometry of nucleic acids containing non-charged non-phosphate linkages and application of this technique to DNA sequencing and mutation analysis  
INVENTOR(S): Gut, Ivo Glynne; Beck, Stephan August  
PATENT ASSIGNEE(S): Imperial Cancer Research Technology Limited, UK  
SOURCE: PCT Int. Appl., 106 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

PATENT NO. KIND DATE APPLICATION NO. DATE

WO 9627681	A1	19960912	WO 1996-GB476	19960304
EP 813609	A1	19971229	EP 1996-904215	19960304
JP 11500924	T2	19990126	JP 1996-526690	19960304
US 6268129	B1	20010731	US 1997-894836	19971124
PRIORITY APPLN. INFO.:			GB 1995-4598	A 19950303
			WO 1996-GB476	W 19960304

AB A method of analyzing a nucleic acid by mass spectrometry comprising the steps of: (1) prepg. a nucleic acid mol. comprising a neg. charged non-phosphate sugar-sugar linkage; (2) eliminating the charge from all, or up to all but ten, of the sugar-sugar linkages of the said nucleic acid mol.; (3) introducing the said nucleic acid mol. in which the charge has been wholly or partly eliminated as said into a mass spectrometer; and (4) detg. the mass of the said nucleic acid mol. Preferably, the nucleic acid has no or one charge. A method of prepg. a nucleic acid mol. contg. no or up to ten neg. charges and no or up to ten pos. charges comprising the steps of (1) synthesizing a nucleic acid with a phosphorothioate linkage or a phosphoroselenoate linkage between sugar residues, and (2) reacting the said nucleic acid with an alkylating agent so as to eliminate the charge on the said phosphorothioate linkage or said phosphoroselenoate linkage. The methods are useful for DNA sequencing and mutation anal., and the nucleic acids are useful to suppress gene expression. Synthetic phosphorothioate-linked oligonucleotides were alkylated, preferably with C<sub>2</sub>H<sub>5</sub>I, and analyzed by both pos.-ion and neg.-ion MALDI. The phosphorothioate DNA was also prepd. in a Sanger-type approach, using .alpha.-S-ddCTP as terminator, for DNA sequence detn. by MALDI. In a third method, phosphorothioate DNA was prepd. by PCR in order to detect mutations by MALDI. Methods for charge-tagging (attaching quaternary ammonium groups to phosphorothioate-linked DNA) were developed. Efficiency of detection of the charge-tagged DNA relative to non-tagged DNA was improved 20-fold.

L1 ANSWER 34 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1996:365110 CAPLUS  
DOCUMENT NUMBER: 125:109297  
TITLE: Synthesis of electrophore-labeled oligonucleotides and characterization by matrix-assisted laser desorption/ionization mass spectrometry  
AUTHOR(S): Britt, Phillip F.; Hurst, Gregory B.; Buchanan, Michelle V.

CORPORATE SOURCE: Chem. Anal. Sci. Div., Oak Ridge Natl. Lab., Oak Ridge, TN, 37831, USA

SOURCE: Journal of Mass Spectrometry (1996), 31(6), 661-668

CODEN: JMSPFJ; ISSN: 1076-5174

PUBLISHER: Wiley

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Recent work to apply mass spectrometric methods to DNA anal. has led to the attachment of an electrophore to an oligonucleotide primer, with the purpose of investigating whether the advantages of electron capture ionization (increased ionization efficiency, reduced fragmentation) could be extended to larger mols., such as Sanger sequence ladders. The stability of the electrophore-modified primers under conditions encountered during matrix-assisted laser desorption/ionization mass spectrometry (MALDI-MS) was investigated. Four different electrophore labels were successfully attached to the 5' terminus of a 17-base, single-stranded oligodeoxyribonucleotide sequencing primer. The attached electrophore tags were robust under conditions used for sample prepn. and MALDI -MS, and little or no fragmentation resulting from loss of the electrophore was obsd. Although no sensitivity enhancement was obsd. for the electrophore-labeled DNA, mass spectrometric conditions are discussed under which the electrophore labels could enhance the detection of DNA sequencing ladders.

L1 ANSWER 35 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1996:355921 CAPLUS

DOCUMENT NUMBER: 125:80968

TITLE: "Detection of single macromolecules using a cryogenic particle detector coupled to a biopolymer mass spectrometer"

AUTHOR(S): *Twerenbold, Damian; Vuilleumier, Jean-Luc; Gerber, Daniel; Tadsen, Almut; van den Brandt, Ben; Gillevet, Patrick M.*

CORPORATE SOURCE: Inst. Phys. l'Universite, Neuchatel, CH-2000, Switz.

SOURCE: **Applied Physics Letters (1996), 68(24), 3503-3505**

CODEN: APPLAB; ISSN: 0003-6951

PUBLISHER: American Institute of Physics

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Macromols. with masses up to 50 kDa were detected with a cryogenic particle detector in a MALDI time-of-flight biopolymer mass spectrometer. The cryogenic particle detector was a Sn/Sn-ox/Sn tunnel junction operated at a temp. of 0.4 K. A calibration with 6 keV single photons inferred that the delayed detector pulses corresponded to the absorption of the kinetic energy of a single macromol. Time-of-flight spectra of lysozyme proteins are presented. The mass resoln. is 100 Da at 14,300 Da. The energy sensitive detection mechanism suggests that cryogenic particle detectors have a high and mass-independent detection efficiency for macromols.

L1 ANSWER 36 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1996:161749 CAPLUS

DOCUMENT NUMBER: 124:255004



TITLE: Investigation of oligonucleotide fragmentation with matrix-assisted laser desorption/ionization Fourier-transform mass spectrometry and sustained off-resonance irradiation

AUTHOR(S): Hettich, Robert L.; Stemmler, Elizabeth A.

CORPORATE SOURCE: Oak Ridge National Lab., Oak Ridge, TN, 37831-6365, USA

SOURCE: Rapid Communications in Mass Spectrometry (1996), 10(3), 321-7

CODEN: RCMSEF; ISSN: 0951-4198

PUBLISHER: Wiley

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Matrix-assisted laser desorption/ionization (MALDI) can be combined with Fourier-transform ion cyclotron resonance mass spectrometry (FTMS) for the detailed structural examn. of biomols. such as peptides and oligonucleotides. We have been able to detect mol. ions for bovine heart cytochrome c (MW = 12 327) by MALDI-FTMS (355 nm laser desorption, 2,5-dihydroxybenzoic acid matrix). Although the mass resolu. of these mol. ions is poor, the expts. verify that the MALDI -FTMS mass range for our 3-T instrument is in excess of  $m/z$  12 000. Accurate mass measurements and selective dissocn. expts. were used to examine the fragmentation pathways of small oligonucleotides in detail. Sustained off-resonance irradiation (SORI) was found to be superior to conventional on-resonance collisionally activated dissocn. (CAD) for the efficient dissocn. and detection of fragment ions for oligonucleotides. These expts. indicated that oligonucleotide fragmentation is a complex process and results not only from simple elimination of nucleic bases and cleavages of phosphate ester bonds, but also by rearrangement processes in which a terminal phosphate moiety can be transferred to an internal phosphate group.

L1 ANSWER 37 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1996:95635 CAPLUS

DOCUMENT NUMBER: 124:169949

TITLE: Characterization of SDS-PAGE-Separated Proteins by Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry

AUTHOR(S): Liang, Xiaoli; Bai, Jian; Liu, Yan-Hui; Lubman, David M.

CORPORATE SOURCE: Department of Chemistry, University of Michigan, Ann Arbor, MI, 48109-1055, USA

SOURCE: Analytical Chemistry (1996), 68(6), 1012-18

CODEN: ANCHAM; ISSN: 0003-2700

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new strategy to characterize SDS-PAGE-sepd. proteins with MALDI MS is described. The proteins, electroblotted onto nitrocellulose after SDS-PAGE sepn. and stained with reversible Ponceau S dye, are readily recovered by dissolving the membrane in matrix solns. prepd. with acetone. The resulting mixts. are amenable to direct MALDI MS anal., which provides a rapid and accurate means of measuring the mol. wts. of SDS-PAGE-sepd. proteins and of peptides that result from CNBr digestion of proteins on the nitrocellulose membrane. Compared with the traditional elution

method, this procedure provides more efficient detection of proteins and peptides, esp. the higher mol. wt. proteins from the membrane. As little as 3.5 pmol of lysozyme and 15 pmol of bovine albumin loaded onto a gel can be detected using this method. The detection sensitivity is higher than or comparable to that of the traditional Coomassie Brilliant Blue staining procedure.

L1 ANSWER 38 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1996:73832 CAPLUS

DOCUMENT NUMBER: 124:163768

TITLE: Strategy for pulsed ionization methods on a sector mass spectrometer

AUTHOR(S): Lennon, John D., III; Shinn, David; Vachet, Richard W.; Glish, Gary L.

CORPORATE SOURCE: Department of Chemistry, University of North Carolina, Chapel Hill, NC, 27599-3290, USA

SOURCE: Analytical Chemistry (1996), 68(5), 845-9

CODEN: ANCHAM; ISSN: 0003-2700

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A method to help facilitate efficient implementation of pulsed ionization methods on a double-focusing sector mass spectrometer is described here. This method involves the addn. of an inductive detector between the elec. and magnetic sectors. The inductive detector will allow a crude, but complete time-of-flight mass spectrum to be acquired with as little as a single laser shot, thereby avoiding the necessity of sequentially compiling limited mass ranges as was done previously. Mass anal. by the complete sector instrument can be performed simultaneously with the time-of-flight anal.

L1 ANSWER 39 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1996:73828 CAPLUS

DOCUMENT NUMBER: 124:140143

TITLE: Matrix-Enhanced Secondary Ion Mass Spectrometry: A Method for Molecular Analysis of Solid Surfaces

AUTHOR(S): Wu, Kuang Jen; Odom, Robert W.

CORPORATE SOURCE: Charles Evans Associates, Redwood City, CA, 94063, USA

SOURCE: Analytical Chemistry (1996), 68(5), 873-82

CODEN: ANCHAM; ISSN: 0003-2700

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new methodol., matrix-enhanced secondary ion mass spectrometry (ME-SIMS), is reported for the mol. anal. of biomaterials. The technique applies static secondary ion mass spectrometry (SSIMS) techniques to samples prepd. in a solid org. matrix similar to sample preps. used in matrix-assisted laser desorption/ionization (MALDI). Mol. ions are obsd. in this ion beam sputtering of org. mixts. for peptides and oligonucleotides up to masses on the order of 10 000 Da. This matrix-enhanced SIMS exhibits substantial increases in the ionization efficiency of selected analyte mols. compared to conventional SSIMS processes. Thus, higher mass peptides, proteins, and nucleic acids become

accessible to near-surface anal. by ion beam techniques, and subpicomole sensitivity has been demonstrated. A no. of matrixes were examd. for their efficiency in ME-SIMS applications, and these initial matrix studies focused on common MALDI matrixes and their isomers. The results of this survey indicate that 2,5-dihydroxybenzoic acid provides the best general enhancement of mol. secondary ions emitted from analyte/matrix mixts.

L1 ANSWER 40 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1996:19880 CAPLUS

DOCUMENT NUMBER: 124:70590

TITLE: Characterization of matrix-assisted laser desorption based on absorption and acoustic monitoring

AUTHOR(S): Preisler, Jan; Yeung, Edward S.

CORPORATE SOURCE: Ames Laboratory-United States Department Energy  
Chemistry, Iowa State University, Ames, IA, 50011, USA

SOURCE: Applied Spectroscopy (1995), 49(12), 1826-33

CODEN: APSPA4; ISSN: 0003-7028

PUBLISHER: Society for Applied Spectroscopy

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Conventional methods for studying matrix-assisted desorption-ionization rely on mass spectroscopy. A 488-nm Ar-ion laser beam is deflected by two acoustooptic deflectors to image plumes desorbed at atm. pressure via absorption. All species, including neutral mols., were monitored. Interesting features, e.g., differences between the initial plume and subsequent plumes desorbed from the same spot, or the formation of two plumes from one laser shot, are obsd. Total plume absorbance can be correlated with the acoustic signal generated by the desorption event. A model equation for the plume velocity as a function of time is proposed. Optical probing also enables accurate detn. of plume velocities at reduced pressures. These results define the optimal conditions for desorbing analytes from matrixes, as opposed to achieving a compromise between efficient desorption and efficient ionization as is practiced in mass spectrometry.

L1 ANSWER 41 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1995:903973 CAPLUS

DOCUMENT NUMBER: 123:334106

TITLE: "Revisit of MALDI for small proteins"

AUTHOR(S): Zhu, Y. F.; Lee, K. L.; Tang, K.; Allman, S. L.; Taranenko, N. I.; Chen, C. H.

CORPORATE SOURCE: Oak Ridge Natl. Lab., Health Sci. Res. Div., Oak Ridge, TN,  
37831-6378, USA

SOURCE: **Rapid Communications in Mass Spectrometry** (1995), 9(13), 1315-20

CODEN: RCMSEF; ISSN: 0951-4198

PUBLISHER: Wiley

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Matrix-assisted laser desorption/ionization (MALDI) was used for several small proteins (such as insulin) and for peptides. The detection efficiencies of MALDI for the insulin B chain and the insulin A chain are drastically different. Similar phenomena were also obsd. for various types of peptides. The pos.-ion signal of MALDI in detecting proteins or peptides was greatly enhanced by the presence of a basic amino acid in their chains. The exptl. results indicate that this enhancement may arise from proton transfer in soln. by an acid-base reaction between the protein/peptide and matrix mol. This pre-protonated mechanism provides a low energy barrier for the ionization of peptides in a MALDI process and greatly reduces the energy threshold of MALDI. Matrix effects on the ionization mechanism are discussed.

L1 ANSWER 42 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1995:40459 CAPLUS

DOCUMENT NUMBER: 122:127051

TITLE: Monitoring protein kinase and phosphatase reactions with matrix-assisted laser desorption/ionization mass spectrometry and capillary zone electrophoresis: comparison of the detection efficiency of peptide-phosphopeptide mixtures

AUTHOR(S): Craig, A. Grey; Hoeger, Carl A.; Miller, Charleen L.; Goedken, Tammy; Rivier, Jean E.; Fischer, Wolfgang H.

CORPORATE SOURCE: Clayton Foundation Laboratories for Peptide Biology, Salk Institute, San Diego, CA, 92138-9216, USA

SOURCE: Biological Mass Spectrometry (1994), 23(8), 519-28

CODEN: BIMSEH; ISSN: 1052-9306

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Matrix-assisted laser desorption/ionization mass spectrometry (MALDI MS) and capillary zone electrophoresis (CZE) were evaluated for monitoring protein phosphatase and kinase reactions in vitro. Varying concns. of peptide C (YHLEKKYVRRDSG), peptide S (YLIEDNEYTARQGA) and kemptide (LRRSALG) mixed with their corresponding phosphorylated peptides, pC, pS and pkemptide, were analyzed. Comparison between the two techniques indicated that MALDI MS was less quant. than CZE, showing a bias towards detection of the unphosphorylated peptide S and kemptide. In terms of sensitivity, the MALDI MS and CZE techniques are comparable. Protein kinase A phosphorylation of kemptide was monitored with both MALDI MS and CZE, whereas alk. phosphatase dephosphorylation of pC could only be monitored with MALDI MS. The absence of inhibition with phosphatase or kinase buffers is a significant advantage of MALDI MS. In contrast to CZE, the MALDI spectra allow identification of the species analyzed by virtue of their mass. The results obtained emphasize the advantage of monitoring enzymic reactions in buffer solns. using MALDI MS compared with CZE.

L1 ANSWER 43 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1994:599998 CAPLUS

DOCUMENT NUMBER: 121:199998

TITLE: Matrix-assisted laser desorption/ionization mass spectrometry for the structural characterization of modified oligonucleotides

AUTHOR(S): Hurst, Gregory B.; Hettich, Robert L.; Buchanan, M.V.; Stemmler, Elizabeth A.

CORPORATE SOURCE: Oak Ridge Natl. Lab., Oak Ridge, TN, 37831-6120, USA

SOURCE: AIP Conference Proceedings (1993), 288(Laser Ablation: Mechanisms and Applications--II), 519-25

CODEN: APCPCS; ISSN: 0094-243X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Matrix-assisted laser desorption/ionization (MALDI) Fourier transform ion cyclotron resonance mass spectrometry (FTMS) and MALDI time-of-flight mass spectrometry (TOFMS) are being used to characterize conditions for the efficient desorption and ionization of normal and modified nucleic acid components. Basic and acidic matrix materials have been evaluated on the TMS and TOFMS. Using MALDI-FTMS at 355 nm, less fragmentation has been obsd. using 2,5-dihydroxybenzoic acid, while more extensive fragmentation is obsd. for basic matrixes, such as 1,5-diaminonaphthalene and 9-aminophenanthrene. Elevation of the cell pressure by the addn. of Ar or CO<sub>2</sub> provides collisional cooling of desorbed ions, resulting in an enhancement of [M-H]<sup>+</sup> and structurally significant high-mass fragment ions. Using MALDI-TOFMS at 337 nm, fragmentation is significantly reduced relative to that obsd. on the FTMS, perhaps as a consequence of the longer times required for FTMS detection. On the FTMS and TOFMS, cluster ions have been obsd. in the neg. ion mode when metal ions are present in the 2,5-dihydroxybenzoic acid matrix. Metal ion addns. and clusters with matrix salts have also been obsd. for dinucleotides. Applications of MALDI-FTMS and MALDI-TOF to the detection of hydroxylated PAH nucleoside adducts are presented.

L1 ANSWER 44 OF 44 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1994:271061 CAPLUS

DOCUMENT NUMBER: 120:271061

TITLE: Matrix-assisted laser-desorption mass spectrometry of homopolymer oligodeoxyribonucleotides. Influence of base composition on the mass spectrometric response

AUTHOR(S): Schneider, Klaus; Chait, Brian T.

CORPORATE SOURCE: Rockefeller Univ., New York, NY, 10021, USA

SOURCE: Organic Mass Spectrometry (1993), 28(11), 1353-61

CODEN: ORMSBG; ISSN: 0030-493X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Matrix-assisted laser desorption/ionization mass spectrometry (MALDI-MS) has the potential for providing a rapid alternative to gel electrophoresis for DNA sequence anal. provided that an intense mass spectrometric response can be obtained from mixts. of DNA fragments contg. up to 300 nucleotides. MALDI-MS has not yet proved viable for such analyses because the MS response falls off rapidly for mixed-base DNA fragments contg. more than 20-30 mols. Previous studies have demonstrated that base compn. is a crit. factor in the MALDI-MS response of oligodeoxyribonucleotides. This paper describes an investigation of the phys. roots of the obsd. influence of base compn. on the

mass spectrometric response, focusing on homopolymer oligodeoxyribonucleotides (dT7, dT10, dT18, dT36, dG7, dG10, dG18, dI18 and dU18) and dT5G5. Forty-eight different matrix compds. were tested for their ability to produce laser desorption masses spectra for such homopolymer oligodeoxyribonucleotides. Considerably stronger mass spectrometric responses were obtained for polydeoxythymidines than from polydeoxyguanosines, polydeoxycytidines and polydeoxyadenosines. Although mass spectral peaks corresponding to dT18 were obsd. from 20 of the matrixes studied, no discernible response was obsd. for dG18 from any of these matrixes. To elucidate the phys. basis for origins of the obsd. differences in response, a no. of factors were investigated including the ionization efficiency, the tendency towards fragmentation and the extent at which the oligodeoxyribonucleotides were incorporated into the matrix crystals.